

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.35 days

Global applicability domain: Outside

Local applicability domain index: 2.92e-01

Confidence level: 9.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.17</div>	<div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 12.5</div> <div>Predicted: 3.26</div>	<div>Image not found</div> <div>1,3-Dimethyl-4-ethylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.89</div>
<div>Image not found</div> <div>2-Ethyl-p-xylene</div> <div>Measured: 12.5</div> <div>Predicted: 3.70</div>	<div>Image not found</div> <div>1-Ethyl-2-methylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 3.88</div>	